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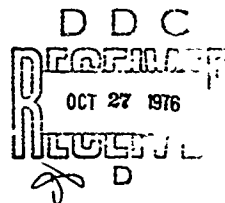
MECHANISMS OF EXHAUST POLLUTANT AND PLUME
FORMATION IN CONTINUOUS COMBUSTION

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Bolling Air Force Base
DC, 20332

UCI Combustion Laboratory
G.S. Samuelson, Principal Investigator



June 1976

SCHOOL OF ENGINEERING

University of California, Irvine
Irvine, California

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An analytical and experimental study is being conducted to promote an understanding of the processes governing the emission characteristics of continuous combustion power sources and thus provide a basis for reducing adverse environmental effects and for controlling plume signatures resulting from aircraft operations. The modeling development can, in addition, be readily adapted to dump combustor and gas turbine combustion. The configuration chosen for the study is an opposed-jet laboratory combustor (OJC). Three numerical programs are used for modeling purposes. The current year has emphasized the		

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utility and range of applicability of the numerical methods for the case of isothermal flow. Eddy viscosity models and boundary condition specification have received the greatest emphasis in a series of systematic test of prediction against experiment. The numerical methods are currently being expanded to include propane as well as methane oxidation kinetics. Evaluation of the numerical codes for the case of hot, reacting flow will be the emphasis of the continuation year. Preheat capability has been added to the experimental dimension of the study. In addition, extensive evaluation of chemical transformation of nitrogen oxides while sampling combustion products is in progress.

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Preface

This second Interim Scientific Report covers the twelve (12) month reporting period, 1 May 1976 to 29 February 1976. The first ten months of the research program were structured to accommodate (1) modification and testing of the experimental system, (2) modification of the numerical methods to the geometry of the opposed reacting combustor, (3) expansion of the numerical methods to include multicomponent reacting flow and, (4) initiation of the cold flow numerical and experimental studies. The current reporting period covers the subsequent twelve (12) month period and includes (1) the test of the numerical methods against experiment for the case of isothermal flow, (2) expansion of the numerical methods to include propane oxidation kinetics in addition to methane oxidation kinetics, (3) expansion of the experimental facility to include air preheat capability, (4) generation of a broad, experimental data base for the cases of isothermal and hot flow, and (5) an in depth exploration of chemical transformations that may occur in probes and lines used to sample and transport nitrogen oxides.

The progress of the second reporting period is presented and accompanied by a description of the progress anticipated for the continuation year.

1. INTRODUCTION

An important category of combustion is designated *continuous combustion* because of a characteristic feature of uninterrupted, chemically reacting backmixed flow. The backmixing serves as a mechanism for flame stabilization. Partially or completely reacted species are backmixed with incoming fresh reactants to provide the energy necessary to sustain the reaction. Power systems that operate on the principle of continuous combustion include gas turbine engines and dump combustors. As shown by the schematic representation of a gas turbine combustor in Figure 1, backmixing of reactive species can be generated down stream of the expansion step (zone B) and at the axis due to swirl imparted to the entering flow (zone A)¹.

1. The Need for Predictive Methods

Engineering design of continuous combustion devices has traditionally focused on overall thermodynamic efficiency, heat transfer rates and power production. Present operating constraints (e.g. exhaust composition and fuel economy) have prompted a more detailed study of the processes occurring within the combustion zone. The more detailed studies can be greatly facilitated by the application of predictive methods to evaluate combustion behavior, and the refined insight provided by point-by-point predictions of concentration, temperature and velocity can be especially valuable. The development of combustion modeling capabilities is also economically advantageous in

that accurate predictions of combustion performance would reduce the need for costly experimental development programs.

The General Problem in Modeling Turbulent Flows. The combustion processes occurring in continuous systems represent a complex interaction of chemical kinetics, heat transfer, mass diffusion and fluid mechanics. The detailed analyses of combustion-chamber flows generally incorporate mathematical sub-models of the chemical and turbulent transport processes in a suitable numerical framework for solving the governing conservation equations. Stemming from the lack of a detailed knowledge to turbulence-combustion interaction, a primary problem in modeling any practical combustion system is to adequately account for the influence of turbulent fluid motions on the heat and mass transfer and on the chemical reaction rates.

The Additional Problem in Continuous Combustion. A characteristic feature of practical continuous combustion systems is a zone of recirculating flow or backmixing. The zone serves as a mechanism for flame stabilization. Partially or completely reacted species are backmixed with incoming fresh reactants, providing the energy necessary to sustain the reaction. As a result, the zone of recirculation is a major factor in determining the overall features of the combustion flowfield and must be carefully considered in the application of modeling methods. To account properly for the zone of recirculation requires solution of the appropriate elliptic partial differential equations rather than the less cumbersome, more extensively investigated parabolic equations applicable when addressing only boundary layer type flows.

1.2 The Need for Experimental Data

Experimental data are required to (1) evaluate and develop the utility and range of applicability of the predictive methods, and (2) to explore pollutant and plume formation in continuous combustion both prior and subsequent to the availability of a suitable predictive method.

The development and evaluation of predictive methods depends upon the design and conduct of a systematic experimental program to provide the data necessary to assess the numerics, boundary conditions, initial conditions, and the submodels of energy and mass transport, and chemical reaction. The most productive approach to resolving the validity, utility, and range of applicability of predictive methods is to perform relevant, well-controlled experiments designed to isolate a single dominant phenomena, and to perform in conjunction with the experiment, simultaneous numerical simulations.² Progress in continuous combustion modeling is currently restricted by the scarcity of detailed flowfield data for distributed reactions with recirculation. Measured profiles of chemical composition, temperature, velocity, and turbulence intensity in backmixed, distributed reactions are necessary to effectively develop and evaluate predictive methods for continuous combustion.

In the absence of a fully evaluated and developed predictive method, the experiment must guide the exploration of pollutant and plume formation in continuous combustion. Though costly and cumbersome in comparison to numerical simulation, experimental studies must currently be

relief upon to provide insight into the performance of these complex systems. Nevertheless, the parallel development and evaluation of predictive methods can greatly enhance the information derived from the experiment.

1.2 the UCI Program

Objectives. The objectives of the UCI program are directed to clarifying the relative influence of those mechanisms responsible for pollutant production in continuous combustion. Specifically the objectives of the study are:

Near Term

- o To investigate high temperature chemical reactions, studying the limits of combustion under those conditions typical of recirculating, turbulent reacting flowfields. Such information is pertinent to combustion stability and use of alternative fuels in turbine, dump, and ramjet combustors.
- o To develop an understanding of pollutant formation in continuous combustion stabilized by recirculation. Such information is pertinent to reducing environmental impact and controlling plume signature.
- o To develop and verify numerical methods and associated submodels of turbulence and kinetics as applied to recirculating turbulent reacting flowfields characteristic of turbine combustion, via a judicious coupling of numerical methods to experiment. The goal is to establish a method that can be readily adopted to the flow geometry of gas turbine, dump, and ramjet combustors.

Future

- o To investigate emission and performance characteristics of alternative fuels with specific emphasis on particulate formation and flame luminosity.

Approach. The UCI investigation of exhaust pollutant and plume formation in continuous combustion is a combined analytical and experimental study of turbulent, backmixed combustion.

Experiments are being conducted using laboratory backmixed combustors operating with premixed and nonpremixed methane/air and propane/air reactants. Operation on liquid fuels is currently being added. Numerical models are being developed and systematically tested against the experimental results to evaluate and improve the models. The goal is to identify, understand, and control pollutant and plume formation in backmixed combustion typical of gas turbine engines.

The investigation is divided into the following elements: The implementation of the elements is detailed in the Performance Schedule presented in Figure 2.

o Model Development and Evaluation

Evaluate and refine numerical procedures and models of turbulence by comparing numerically predicted profiles of velocity, turbulence energy, temperature, and tracer concentration of experimentally determined profiles (nonreacting and reacting flow).

Evaluate and refine the numerical procedures and the coupled models of turbulence and chemical kinetics by comparing numerically predicted profiles of velocity, turbulence energy, temperature, tracer concentration, and mass fractions of hydrocarbons, nitric oxides, carbon monoxide, oxygen, and carbon dioxide to experimentally determined profiles (reacting flow).

o Mechanisms of Pollutant/Plume Formation

Perform parametric studies (theoretical and experimental) to identify the relative contribution of the chemical reactions, transport processes (heat and mass diffusion, fluid mechanics, and recirculation behavior), and system parameters (e.g. geometry flow rates) to pollutant formation.

o Supplemental Studies

Lean Combustion. Evaluate the emission characteristics of the opposed jet combustor (OJC) and the potential of utilizing the OJC in stabilizing lean combustion.

Swirl. Design and install the capability to generate and control swirl in the laboratory combustor systems.

Air Preheat. Install the capability of a r preheat to 600°C to more effectively simulate gas turbine combustion behavior.

Non-Premixed Combustor. Expand the existing premixed combustion studies to include non-premixed systems more representative of the majority of gas turbine systems.

Particulate Formation/Luminesity. Investigate particulate formation in reacting flows with recirculation with special emphasis on alternative fuels. Investigate luminosity in reacting flows with recirculation with special attention to alternative fuels and impact on combustion liner degradation.

NO Probe. Explore chemical transformation of nitrogen oxides in sample probes and sample lines while sampling combustion products. Such information is important in the use of measured concentration data in pollutant and plume formation studies.

1.4 The UCI Combustor Systems

Two combustor systems--premixed and nonpremixed--are employed in the UCI study. Schematics of both systems are presented in Figure 3. The premixed system, shown in Figure 3a, is an opposed-reacting-jet combustor (OJC). The non-premixed system, shown in Figure 3b, is a classical configuration with fuel injected at the axis in a stream concurrent with the surrounding air.

The opposed-jet combustor (OJC) exhibits essential features found in practical continuous combustion systems (backmixing, high intensity combustion) but avoids the attendant complexities (nonpremixed, two phase combustion) appropriate for complementary studies. The recirculation zone is isolated and free from geometrically governed boundary conditions.

The isolation allows the turbulent/hydrodynamic effects to be explored apart from the complicating questions associated with boundary condition specification. The features of the OJC especially attractive and novel to the study are the extended range and control of turbulence intensity, mixing lengths, and mixture equivalence ratios versus those offered by the sudden expansion on physical, bluff body configurations. For example, the rate and intensity of backmixing in the recirculation zone may be altered experimentally and numerically over a broad range by varying the ratio of approach velocity to jet velocity.

The OJC combustor is a 51mm I.D. x 457mm cylindrical Vycor chamber containing an aerodynamic (opposed-jet) flame-holder. The incoming flow of premixed fuel (methane or propane) is opposed by a high velocity jet ($\dot{m}_j/\dot{m}_m \ll 1$) issuing from a 1.3mm I.D. (6.4mm O.D.) water-cooled tube. The jet is coincident with the combustor axis and located 76mm upstream from the combustor exit. The backmixed zone required for flame stabilization is generated along the jet boundary. The combustor is currently being enlarged to 78mm to improve the resolution of the flowfield spatially.

The nonpremixed system is currently being designed. The combustor size will match the expanded premixed version of 78mm. The nonpremixed configuration will allow exploration of the effects of mixing the two dissimilar streams on pollutant formation and numerical prediction, allow utilization of liquid fuel, and provide a bridge between the premixed system and the more conventional turbine combustor configurations.

2. BACKGROUND

2.1 Numerical

The development of a predictive method for continuous combustion must be founded upon a suitable computational procedure. Because the flows are characterized by strong back-mixing, the describing partial differential equations must be elliptic.

A computational technique may be developed to solve the elliptic equations wherein the goal is to solve directly for the instantaneous velocity. This approach is costly, relatively complex, and requires substantial computer storage capacity. An alternative approach for engineering calculations is to adopt time-averaged properties. Here, instantaneous properties (pressure, temperature, velocity....) are replaced by the sum of the mean (time-averaged) value of the property and a fluctuating component. The governing equations are then structured in terms of the time-averaged properties plus additional terms involving the fluctuating components. The problem, then, is transformed from solving for the time-dependent instantaneous velocity to providing a model that accounts for the new fluctuating component terms in the time-averaged equations.

One approach used to account for the fluctuating component terms is to modify the transport properties (e.g., viscosity, μ). The modified values of the transport properties are called effective properties (e.g., effective viscosity, μ_{eff}) and

formulated to account for the turbulence transport associated with the fluctuating components. Examples of two effective viscosity models are the following algebraic and two-equation formulations:

Algebraic³

$$\mu_{\text{eff}} = K D^{2/3} L^{-1/3} \rho^{2/3} (\bar{u}V^2)^{1/3} \quad (1)$$

K: empirical coefficient
 D: diameter of combustor
 L: length of combustor
 ρ : local density
 $\bar{u}V^2$: inlet kinetic energy

Two-Equation⁴

$$\mu_{\text{eff}} = c_{\mu} \rho k^2/\epsilon \quad (2)$$

c_{μ} : empirical coefficient
 ρ : local density
 k : local turbulent kinetic energy
 ϵ : local turbulent energy dissipation rate

For a given geometry and inlet flow rate, the algebraic formulation is functionally dependent only upon local density. The two-equation model introduces additional unknowns that complicate the numerics and adds computational cost penalties. However, the two-equation effective viscosity model is

intuitively more accurate because it accounts for spatial variations in turbulent kinetic energy and length scale.

The turbulent transport of scalar quantities is related to the eddy viscosity through the appropriate Prandtl or Schmidt numbers as follows:

$$\Gamma_{\text{eff},\phi} = \frac{\mu_{\text{eff}}}{\sigma_{\text{eff},\phi}} \quad (3)$$

Γ_{eff,ϕ : effective exchange coefficient for dependent variable ϕ

σ_{eff,ϕ : Prandtl or Schmidt number

ϕ : dependent variable

Table I lists the following major computer codes that have been developed using the time-averaged approach to solve the elliptic flow equations:

PISTEP II is a ψ - ω program with a two-equation effective viscosity model. The UCI version includes combustion chemistry, the OJC geometry, and the algebraic description of effective viscosity for convenience in initiating a first solution.

TEACH is a three-dimensional program written with p - v as the major, dependent variables. The code has the attractive features of a third dimension option and an efficient iterative routine. The UCI version includes both a two-parameter and algebraic description of the eddy viscosity models as well as the combustion chemistry, and OJC

geometry

A third code, CRISTY, developed at United Technology Research Center (UTRC) through a joint sponsorship by the Environmental Protection Agency (EPA) and the Air Force Aero Propulsion Laboratory (AFAPL), is being run in cooperation with the EPA.

2.2 Experimental

The experimental dimension of the UCI program combines the following components of the continuous flow combustion test facility in the UCI Combustion Laboratory:

- combustor test facility
- gas analysis system
- laser velocimeter

The integrated system represents the unique experimental capability of providing detailed measurements of composition, temperature, velocity and turbulence data to (1) develop and evaluate the predictive methods, (2) explore the mechanisms of exhaust pollutant and plume formation, and (3) conduct supplemental studies.

Combustor Test Facility. The test facility includes built-in controls and measuring devices for monitoring operating parameters as well as diagnostics for the flame and emission characteristics. Provisions are included for varying operational parameters continuously while the combustor is firing. The structural features of the combustor test section

readily accommodate mechanical probing for sample input to the gas analysis system and optical probing by the laser velocimeter. Combustor air inlet temperatures up to 600°C (1112°F) can be accommodated. A flow diagram of the test facility is shown in Figure 4. The combustor test section is nominally 51mm in diameter and is currently being expanded to 78mm. The air is supplied on a continuous basis (0.1Kg/sec) with approach velocities variable to 18.3 meters/sec (60 ft/sec).

The combustor facility is interfaced with an automated data acquisition system coupling an analog data scanner with a minicomputer. System capabilities include real-time monitoring and control of the experiments and efficient data reduction. A block diagram of the data acquisition system is shown in Figure 5.

Gas Analysis System. A packaged turbine engine analysis system (Scott Research Labs., Model 113) is available for the exhaust gas analysis. The unit consists of five commercially available instruments: Two nondispersive infrared analyzers (NDIR) for measurement of CO and CO₂, a chemiluminescent analyzer (CLA) for measurement of NO/NO_x, a flame ionization detector (FID) for total hydrocarbons, and a paramagnetic oxygen analyzer. Also included is the associated peripheral equipment necessary for sample conditioning and instrument calibration. All instruments supply an analog output to a 5-channel strip chart recorder and/or the data acquisition systems. A detailed breakdown of the analytical instruments is shown in Table II.

Laser Velocimeter. A DISA type 55L laser Doppler velocimeter (LDV) system is available for velocity measurement in the combustor flowfield. The principal components of the LDV system include a 5 mW He-Ne laser light source manufactured by Spectra-Physics (Model 120) an integrated optical unit and a DISA (Model 55L20) frequency tracker for Doppler signal processing. The signal processing is currently being expanded to include frequency counting through use of the PDP-11 computational and data sampling capability.

The LDV optical bench is mounted on a motorized traverse to facilitate rapid scanning of the flowfield while maintaining an accurate spatial resolution. A schematic diagram of the LDV optical arrangement and associated electronics is shown in Figure 6.

In our experience to date, it has been found necessary to artificially seed the flow system with supplementary light scattering particles to provide an adequate signal input to the data processing instrumentation. The nonreacting flow studies are conducted using salt (NaCl) particles introduced into the flow as an aerosol. Combustion experiments necessitate introducing high melting point solids, such as alumina Al_2O_3 , by a fluidized bed technique.

2.3 Coupled Numerical/Experimental Procedure

The program plan of the investigation is designed to accomplish the objectives of the study via a judicious coupling of numerical methods to experiment. The approach is to address in sequence isothermal (nonreacting), heated (nonreacting with

preheat), and hot (reacting flow). The approach is outlined in Table II and illustrated in Figure 2. The eddy viscosity and mass transport submodels, and initial conditions and boundary conditions are first tested against experiment for isothermal flow. The tests used include comparisons of velocity profiles, turbulence intensity profiles, and profiles of tracer concentrations. The eddy viscosity, mass transport, and energy transport submodels, and initial and boundary conditions, are secondly tested against experiment for heated (nonreacting) flow. The main stream and jet stream are independently heated to temperatures in excess of 400°C (754°F). The tests used include comparisons of velocity profiles, turbulence intensity profiles, profiles of tracer concentration, and temperature profiles. Third, the eddy viscosity, mass transport, energy transport, and chemistry submodels, and initial and boundary conditions are tested against experiment for hot (reacting) flow. The tests include those above plus comparison of species concentration profiles of the major products of combustion as well as carbon monoxide and oxides of nitrogen.

The rate and intensity of backmixing in the recirculating flow region are altered numerically and experimentally by variations of the ratio of approach velocity and jet velocity. Turbulence intensity and scale (eddy size) are altered by the use of screen grids upstream of the stabilization zone. The comparative tests encompass a broad range of turbulent transport rates between the recirculation zone and the primary gas stream. Additional parametric variations include the mixture equivalence ratio.

2.4 NO Probe

Measurement of combustion products in laboratory burners and flames is required to identify the elements of chemical kinetic and fluid mechanics responsible for the formation of pollutant species.

Measurement of the gaseous product composition emitted from a combustion source generally proceeds by extracting an exhaust sample for subsequent quantitative analysis. In order to obtain reliable data, precaution must be taken to ensure that the analytical instrumentation receives a sample that is chemically identical to the composition existing at the sampling point. Potential sample transformations may be minimized by careful selection of materials contacting sample gases in the physical probe used for sample removal and in the line used to transport the sample to the instrumentation.

Of all the significant products of combustion, nitrogen oxides (NO_x) are especially susceptible to chemical transformation. In addition to the total nitrogen oxides concentration, the concentration of the primary species in the nitrogen oxides family, nitric oxide (NO) and nitrogen dioxide (NO_2), must often be determined. For example, spatial distributions of nitric oxide (NO) and nitrogen dioxide (NO_2) are required to identify the chemical kinetic mechanisms responsible for the formation of nitrogen oxides in flames or gas turbine combustors. The oxidation of NO to NO_2 or the reduction of NO_2 to NO in

sample probes and sample lines prevents an accurate determination of either NO or NO₂. As a result, oxidation or reduction reactions involving NO or NO₂ may often be unacceptable even though total NO_x is conserved.

An adequate accounting of NO_x transformations requires that experiments be conducted to identify (1) the chemical transformations, if any, that occur, (2) the extent to which they occur during typical sampling times, and (3) the conditions (e.g. sample temperature, sample composition, sample line material) for which they occur.

The present experimental study is designed to assess NO_x transformations that may be encountered when sampling within flames and at the exhaust plume of laboratory combustors. The experimental system is currently designed to simulate the actual conditions experienced in sample lines used for sampling gaseous combustion products. A diagram of the experimental system is shown in Figure 7. Test parameters include composition of the carrier gas, dopant gases, and probe material.

A carrier gas simulating the primary combustion products is selected from one of three prepared sources of 0, 1, or 5% O₂, 12% CO₂, and balance N₂. The carrier gas flow, 4 liters/minute, is doped with CO, NO, and NO₂ metered from high concentration source cylinders by means of porous sintered metal flow restrictors. After doping, the carrier gas enters a silica preheat tube that raises the gas temperature to the desired probe test temperature. From this point, the doped carrier gas enters a sample probe test section. An oven is used to maintain the temperature of the doped carrier gas at the desired probe test temperature.

The temperature of the gas within the sample probe is incrementally varied from 25°C to 400°C. Temperatures of the gas stream (T_2 and T_3) are measured with insulated platinum resistance thermometers centered in the probe bore at the inlet and outlet of the sample probe. The oven temperature is also recorded by a thermocouple located adjacent to the outer diameter of the sample probe. The sample probe heater can accommodate a variety of probe materials of lengths up to 2 meters.

Gas composition is measured at sample Point 3 to assess the extent of NO and NO₂ transformation within the 2 meter sample probe segment. Sample lines leading from points 2 and 3 (Figure 7) are short, equal-distant, and made of 1/4 inch o.d. TFE Teflon. Screening tests using varying lengths of TFE Teflon have been conducted to assure that NO₂ absorption is not a significant factor in the present experiment.

Analysis of NO and NO_x is conducted with a Beckman Model 951H chemiluminescent oxides of nitrogen analyzer. NO₂ is determined by the difference between the measured NO_x and NO concentrations. The (carbon) converter efficiency is monitored by periodic tests using the methods outlined in the Federal Register.⁵ Measurements of carbon monoxide concentration is conducted with a Beckman Model 315BL nondispersive infrared analyzer.

3. DESCRIPTION OF PROGRESS; REPORTING PERIOD

The performance schedule is presented in Figure 2. The first ten months of the research program were structured to accommodate (1) modification and testing of the experimental system, (2) modification of the numerical methods to the geometry of the opposed reacting combustor, (3) expansion of the numerical methods to include multicomponent reacting flow and (4) initiation of the cold flow numerical and experimental studies.

The current reporting period covers the subsequent twelve (12) month period and includes (1) the test of the numerical methods against experiment for the case of isothermal flow, (2) expansion of the numerical methods to include propane oxidation kinetics, (3) expansion of the experimental facility to include air preheat capability, (4) initiation of the generation of a broad, experimental data base for the cases of isothermal and hot flow, and (5) initiation of an in-depth exploration of chemical transformation that may occur in probes and lines used to sample and transport nitrogen oxides.

The program is on schedule.

3.1 Numerical

A summary of the improvements and modifications completed during the current reporting period is outlined in Table IV. Current problems outstanding and plans for their resolution are

also identified.

PISTEP II and TEACH were tested against experiment for the case of isothermal flow. The results of the TEACH evaluation are discussed in Section 3-3 (Combined Numerical/Experimental) and will be presented at the Sixteenth Symposium (International) on Combustion. The PISTEP II evaluation is currently being completed.

In cooperation with the EPA, the CRISTY Code was modified to the UCI OJC geometry and is currently being run for the algebraic eddy viscosity model.

Solutions have been obtained for hot (reacting flow) mixtures of methane/air with nitric oxide formation using TEACH. Solutions are now being pursued with PISTEP II. Both codes are undergoing modifications to consider propane oxidation kinetics.

In summary, PISTEP II, TEACH, and CRISTY are specialized to the OJC geometry, and are now being tested for the case of isothermal conditions. The evaluation of the methods for the case of hot flow has commenced. The codes are being expanded to include propane kinetics as well as methane oxidation chemistry. Tests of the codes for the hot flow condition will continue during the continuation year.

3.2 Experiment

Combustor Test Facility. A summary of all the improvements and modifications completed during the current reporting period are outlined in Table V. Current problems outstanding and plans

for their resolution are also identified.

The major modification to the combustor test facility was the inclusion of air preheat capability to 600°C (1112°F). Electric heating was selected (1) to avoid contamination of the combustor inlet air (contamination of the inlet air could significantly alter the combustion process chemistry), (2) to provide a precise control of temperature, and (3) to allow a rapid response to changing flow conditions.

The combustor air preheat system is designed to have the flexibility to heat the combustor inlet air to any temperature within the design temperature range and to be operational for a range of airflows. The maximum design temperature for the air preheat system is 600°C. Selection of this temperature is based on actual gas turbine operating conditions. The air preheat system will provide heated inlet air for combustor air velocities of 7.62 to 15.24 m/sec (25 to 50 feet/sec).

The initial series of combustor preheat studies will involve the premixed combustion of propane with heated air. The ignition temperature for a fuel-oxidant mixture is the temperature at which self sustained combustion will occur. Reported ignition temperatures for propane-air mixtures range from 450°C to 600°C. To avoid the possible hazardous condition of mixing propane with air heated to the ignition temperature, a maximum

operating temperature of 400°C will be observed. This maximum temperature will allow combustor studies to be performed at temperatures typical of low pressure-ratio gas turbine engines. Future combustion studies using a nonpremixed combustor configuration will allow the maximum combustor air preheat system temperature to be extended to the desired limit of 600°C.

Laser Velocimeter. The LDV development has emphasized isothermal flow conditions. A commercially available nebulizer is used to introduce supplementary laser light scattering particles into the flow. The nebulizer atomizes high concentrations of uniform size, salt-water solution droplets. The aerosol is dried to small, solid salt particles of uniform size before entering the combustor. The size of the particles is controlled by the original salt concentration in the solution.

Current problems outstanding concern signal acquisition in the recirculation zone and the stress layer located along the periphery of the opposed jet. Several approaches are currently being investigated to improve data acquisition and interpretation. Emphasis is being placed on development of a period timed (counter) signal acquisition system to complement the current frequency tracking technique.

3.3 Coupled Experimental/Numerical

One of the important elements of the current research program is the coupling of the numerical and experimental components. The development of a realistic numerical model of

continuous combustion requires careful validation by way of experimental observation.

Emphasis during the current reporting period has been directed to (1) testing the numerical methods for the case of isothermal flow (to evaluate the eddy viscosity model) and, (2) testing the numerical methods for the case of isothermal flow with a tracer. For the case of isothermal flow, the eddy viscosity submodels were first evaluated for the prediction of system hydrodynamics. A tracer gas was later introduced to evaluate the eddy viscosity submodels for nonuniform, multi-component flow where mass as well as momentum exchange is important. Experimental measurements and numerical predictions of velocity and tracer isopleths for a range of approach velocities and backmix characteristics provided the critical tests.

The results reported here emphasize the case of isothermal flow. A satisfactory assessment and understanding of the isothermal case is a prerequisite to engaging the hot flow case. Combustion imposes the additional requirement for submodels of chemistry and turbulence/chemistry interaction that may mask fundamental deficiencies in the eddy viscosity submodel. However, hot flow results are presented as an indication of the suitability of the two eddy viscosity submodels in the prediction of reacting flows.

The isothermal and hot flow results collectively demonstrate the merits of two eddy viscosity submodels for the prediction of transport behavior in continuous combustion systems of

practical engineering interest (turbulent reacting flows with recirculation). In addition, the results provide useful information for the development of applied computational tools for analyzing the performance of continuous combustion systems.

The present study explores specification of the eddy viscosity, μ_{eff} and turbulent mass transport, $\Gamma_{eff,\phi}$, in confined flows exhibiting strong backmixing or recirculation. Comparative calculations were performed using two distinct turbulence submodels to define the eddy viscosity--an algebraic model (Equation 1) and a more elegant two-equation submodel (Equation 2).

RESULTS (ISOTHERMAL FLOW)

To effectively test the submodels of eddy viscosity over a range of turbulent conditions, experimental data were obtained for approach velocities of 15.24 and 7.62 m/sec and jet velocities of 30.5, 61 and 130m/sec. Velocity profiles were mapped throughout the flowfield using a 1mm O.D. pitot tube. Tracer profiles were generated by introducing alternatively pure carbon monoxide (CO) in the jet and pure carbon dioxide (CO₂) in the mainstream. The mixing between the jet and mainstream was assessed by mapping CO and CO₂ profiles throughout the flowfield using a 3mm stainless steel tube and Beckman 315B NDIR instruments for the gas sampling and analysis. The Reynolds number of the approach stream ranged from 2.5×10^4 (at 7.62m/sec) to 5.0×10^4 (at 15.24m/sec).

Momentum Transport

The eddy viscosity submodels were first tested for a homogeneous, isothermal flowfield to explore the effectiveness of the submodels in predicting momentum transport. Experimental and predicted profiles of the axial component of mean velocity are presented in Figure 8 for an average inlet velocity of 15.24m/sec. The selected profiles emphasize the flow regime dominated by recirculation. The calculated velocity profiles for both turbulence submodels assume an experimentally determined velocity profile as an inlet condition.

The trend of the velocity profiles agrees qualitatively with the experimental results. The two-equation submodel retains the inlet turbulent velocity profile in the approach section while the velocity profiles predicted by the algebraic submodel flatten out due to the spatially uniform viscosity. The presence of the opposing-jet is communicated further upstream for the two-equation submodel than for the algebraic eddy viscosity, and the two-equation submodel demonstrates better correlation with the experimentally observed stagnation point.

The mean velocity profiles in the recirculation zone are also better represented by the two-equation turbulence submodel, although both submodels over-predict the jet expansion. In addition, the two-equation velocity profiles decrease too rapidly near the chamber wall. Downstream from the backmixed zone both submodels fail to adjust for the redistribution of the bulk flow in the turbulent wake of the recirculation zone and under-predict the velocity adjacent to the jet wall. Both submodels display good agreement in the bulk flow regime in the absence of recirculation or wall effects.

The recirculation zone strength was examined by reducing the approach velocity by a factor of two while retaining the same jet velocity. The experimental and predicted velocity profiles are presented in Figure 9. The calculated results demonstrate a significant departure from experiment in the region of strong backmixing. The reverse flow region again penetrates further upstream in the two-equation submodel prediction.

The acceleration of the bulk flow around the recirculation zone is under-predicted in contrast to the over-predicted jet expansion for both submodels. This result is especially evident near the plane of the jet exit where the redistribution of the bulk flow with the jet discharge is restricted. This effect is conveyed downstream from the recirculation zone where the two-equation velocity profiles correlate well with experiment near the chamber wall but deviate near the jet wall.

Mass Transport

The two eddy viscosity submodels were secondly tested in conjunction with the turbulent mass exchange submodel (Eq. 3) for the conditions of an isothermal, nonhomogeneous flowfield. Spatial distributions of the predicted tracer concentrations are compared to experimental measurements in Figures 10 and 11 for the baseline conditions outlined previously.

Figure 10 presents the algebraic and two-equation submodel predictions, and experimental tracer concentration distributions for a 15.24m/sec average inlet velocity. (The jet stream is 100 percent carbon monoxide.) Immediately evident is the contrasting axial and radial spread of the predicted tracer concentration profiles. Differences in axial transport of CO are consistent with the observations forwarded in the previous section on momentum transport. More notable are the diverse radial transport pre-

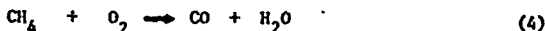
dictions. The spreading of the jet discharge into the mainstream for the algebraic eddy viscosity conforms to the experimental results.

In contrast, the two-equation submodel limits the radial mixing of the jet stream (tracer) with the bulk flow. The segregation of the jet and the mainstream is verified by the high CO concentrations along the jet wall, in contrast to the absence of CO near the chamber wall. This result was further substantiated by introducing a carbon dioxide (CO₂) tracer in the approach stream. The numerical analysis of CO₂ concentrations for the two-equation submodel predict negligible mass transport of CO₂ from the mainstream into the recirculation zone. Downstream, the predicted mixing of CO₂ from the bulk stream into the flow associated with the jet stream is minor. Experimentally CO₂ was observed to be well mixed into the jet.

The results for the strong recirculation zone (Figure 11) demonstrate similar trends. Although the velocity data presented earlier in Figure 9 gave poorer agreement for conditions of strong recirculation, the mixing is improved because of the enhanced backmixing.

RESULTS (HOT FLOW)

A two-step global reaction mechanism for methane oxidation was adopted for the present study to illustrate the applicability of current numerical methods to the prediction of continuous combustion flows, and to briefly explore the suitability of the eddy viscosity submodels for the case of hot flow:



A detailed description of the numerical formulation of the reaction rate expressions and boundary conditions may be found elsewhere⁶. The dependent variables for the hydrocarbon system include the mass fractions Y_{CH_4} and Y_{CO_2} . Distributions of the other major species--water (H_2O), oxygen (O_2), carbon monoxide (CO)--are related to Y_{CH_4} and Y_{CO_2} by elemental mass conservation. An initial solution for the reacting flowfield was obtained using published reaction rates⁷ which were later refined to more closely resemble the experimental data. This approach was justified on the basis that the reaction rate data were obtained from the study of a well-stirred reactor and may not apply to the current study, which deviates substantially from well-stirred conditions. Global reaction rates were judged acceptable for the present study because of the uncertainties encompassing the specification of the system aerodynamics.

Since the aim of the study is to predict the performance of backmixed combustion systems, the hot flow calculations were extended to include the prediction of the pollutant species, nitric oxide (NO). Nitric oxide kinetics were based on the familiar Zeldovich⁸ mechanism:



Noting that reaction (6) is the rate limiting step and adopting the simplifying assumption of O/O_2 equilibrium results in the reaction rate expression:

$$\frac{d[NO]}{dt} = 2 k_{8f} K_O [N_2][O_2]^{\frac{1}{2}} \quad (8)$$

The temperature and O_2 distribution obtained from the solution of the

hydrocarbon system was used as a basis for the NO kinetic calculations.

The experimental tests conducted to complement the numerical predictions of hot flow properties utilized stoichiometric proportions of premixed methane and air in both the main and jet streams. The reactants were initially at ambient temperature and the combustion was completed at atmospheric pressure. The test matrix included the same approach velocities selected for the isothermal cases -- 7.62 and 15.24m/sec -- and a jet velocity of 130m/sec. Detailed maps of flowfield properties were obtained by conventional probing techniques. Temperature measurements were made using an uncoated Pt/Pt-13% Rh thermocouple and a Scott Model 125 chemiluminescent analyzer was used for oxides of nitrogen measurements. Gas samples were extracted via a moveable 3.2mm O.D. watercooled, 316 stainless steel probe having a tubular inlet, and conveyed through a heated teflon sample line to a packaged exhaust gas analysis system. Selected results of hot flow properties are presented in Figures 12 and 13 for the conditions indicated. Temperature and NO profiles are presented as indicators of useful design information that may be derived from the numerical simulation of back-mixed combustion processes.

DISCUSSION

Isothermal Flow

The results of the momentum and mass transport studies identify several important characteristics of the turbulence submodels. The turbulent viscosity from the two-equation submodel varies through the flowfield as is physically expected. The two-equation submodel demonstrates the generation and dissipation of turbulence kinetic energy near the jet exit, the stagnation point, and near the boundaries. In contrast, the

viscosity from the algebraic submodel is spatially uniform throughout the flowfield for isothermal flow, and varies only with a change in the kinetic energy of the inlet streams. The impact of these differences between the two eddy viscosity submodels is evidenced by the velocity profiles, the predicted location of the stagnation point, the radial mass transport, and the dissipation of the kinetic energy of turbulence in the wake region.

Velocity Profiles. The predicted velocity profiles agree qualitatively with experimental results. The two-equation submodel more closely approximates the experimental trends although the predicted velocity contours for conditions of strong recirculation are quantitatively incorrect throughout the flowfield for both turbulence submodels. The departure from experiment is especially evident near walls, and suggests the need to refine the wall functions used to specify boundary conditions for turbulent kinetic energy or dissipation rate, and/or to decrease the grid spacing near the wall.

Stagnation Point. The location of the stagnation point as indicated by the velocity profiles and upstream extent of tracer measurements is better described by the two-equation submodel. The effective viscosity predicted by the algebraic submodel is spatially uniform throughout the flowfield for given inlet conditions. No account is made for changes in the kinetic energy of turbulence or energy dissipation rate in the region of encounter between the main and jet flows. The lower viscosity predicted in the recirculation zone by the two-equation submodel is more effective in describing the actual axial momentum and mass exchange.

Radial Mass Transport. Although the experimentally determined tracer isopleths are in closest agreement in the recirculation zone for the two-equation submodel, the downstream radial spread is more effectively

described by the algebraic submodel. The uniformly high viscosity predicted by the algebraic turbulence submodel aids the overall mass transport throughout the flowfield, i.e. axial and radial diffusion from the jet is greater for the algebraic rather than for the two-equation submodel.

The radial mass transfer predicted by the two-equation turbulence submodel suggests that the principal mechanism of mass transport is by large-scale convection rather than by small scale gradient diffusion processes.¹⁰ The tracer concentration varies gradually through the recirculation zone. The downstream mixing layer is bounded by steep concentration gradients that enclose the jet mixing region. The numerical predictions indicate that at high approach velocities the bulk flow detours around the recirculation zone, retaining upstream flow properties (low viscosity and small-scale mixing) and effectively precludes radially-directed mass transport. Conversely, the experimental trend reinforces the conjecture that turbulent exchange processes should be active downstream from the recirculation zone.

Wake Region. The kinetic energy of turbulence predicted by the two-equation submodel is quickly dissipated in the wake region downstream of the recirculation zone. The resulting low viscosity impedes turbulent mixing throughout the wake region. In contrast, the uniformly high viscosity of the algebraic submodel is effective in predicting the radial spread of tracer observed experimentally.

Hot Flow

The hot flow results reflect the inherent limitations of the underlying eddy viscosity submodels and emphasize the urgency to refine the basic fluid dynamic representations employed in the analytical models.

In general, the predicted hot flow properties qualitatively simulate gross flame features. Before adequate experimental correlation is achieved, however, the submodels of eddy viscosity and turbulent mass exchange must perform satisfactorily for the case of isothermal flow, and the chemical submodels and the coupled turbulence/chemistry interaction must be fully explored and likely improved for the case of hot flow.

Refinement

The results above identify directions for refinements to the eddy viscosity submodels, inlet conditions, and/or surface boundary conditions. A parametric investigation was initiated to improve the predictions of the two-equation eddy viscosity submodel by exploring the effect of boundary condition specifications.

The outcome of the parametric studies suggested that in confined flows, where the recirculation zone may contact solid boundaries, the specification of near wall turbulence energy dissipation rate (ϵ) may significantly influence the mixing characteristics of the two-equation turbulence submodel. These results are consistent with the findings of earlier studies¹¹ where a reduction of ϵ adjacent to a downstream facing wall was used to improve numerical/experimental correlation. Similarly, the reduction of ϵ on the upstream facing step of the jet tube was found to radically alter the predicted mass transport behavior of the two-equation submodel. The improved radial mass transport is evidenced by the tracer concentration profiles in Figure 14 with a slight sacrifice in stagnation point correlation. The stagnation point correlation can be improved by modifying k or ϵ at the jet inlet.

The refinements clearly demonstrate the sensitivity of the numerical solution to boundary condition specification, and the need to test the two-equation turbulence submodel under isothermal flow conditions prior to hot flow simulations.

CONCLUSIONS

Numerical predictions of the turbulent, backmixed flowfield of an opposed-jet combustor have been compared to experimental observations. Although favorable qualitative correlation has been established, deficiencies in the eddy viscosity submodels and associated boundary conditions used as a foundation for the transport mechanisms have been identified.

The flowfield hydrodynamics are more accurately represented by the two-equation submodel because of the intrinsic variable viscosity and length scale. Comparable solutions may be obtained at considerably less expense by employing the algebraic submodel.

The mass transport predictions of the algebraic submodel demonstrate acceptable correlation. The prediction of radial mass transport by the two-equation submodel in general does not conform to experiment. The performance of the two-equation submodel may be improved by careful specification of boundary conditions. In particular, the near wall turbulence energy dissipation rate was shown to significantly influence the mixing characteristics of the two-equation submodel.

The results of the isothermal flow studies indicate that the algebraic turbulence submodel performs adequately in describing general fluid flow patterns and mass transport for the conditions investigated.

A major impact of the present study is that considerable testing of the numerical model is required for isothermal flow before proceeding to the complicating conditions of combustion. The testing requires a coupled numerical/experimental study and is likely governed by the geometry, inlet and solid boundary conditions of the system under investigation. The hot flow calculations presented here accentuate the inadequate transport characteristics identified in the isothermal flow analysis. Attempts to refine the chemistry submodel or to quantify the interaction of fluid motions on chemical reaction rates are dependent on the correct turbulence model formulation.

3.4 NO Probe

Effects of oxygen containing, and carbon monoxide containing atmospheres on nitrogen oxides concentration were evaluated during the current reporting period. Sample probe materials tested included 304, 316, and 321 stainless steel and silica. The length of each sample probe was arbitrarily chosen to be 2 meters. The residence time of the doped carrier gas in the sample probe test section was approximately 1 second for the 4 liters/minute flow rate and 2 meter sample probe length.

The NO and NO₂ input levels to the sample probe (Sample Point 2 in Figure 7) were chosen to be 500ppm and 75ppm respectively. These levels simulate NO concentrations which are typically encountered in sampling and a NO₂ concentration which is thought to be representative. CO levels selected were 0, 100, 1000, and 2500ppm.

The results are presented in Figure 15 for mixtures without carbon monoxide and in Figure 16 for mixtures with carbon monoxide. The percent change of NO and NO₂ represent the percent change in concentration between Sample Points 2 and 3 (Figure 7). Since total NO_x was conserved in all cases, the figures demonstrate a direct correspondence between NO and NO₂ transformations. The temperature shown is the gas temperature at Sample Points 2 and 3. The results without carbon monoxide were presented at the First International Chemical Congress in the Western Hemisphere in December, 1975.¹² The results with carbon monoxide were presented at the Western States Section of

the Combustion Institute in April, 1976.¹³

RESULTS (WITHOUT CARBON MONOXIDE)

The results for silica are presented in Figure 15a. No significant transformation is observed over the temperature range and the residence time studied. Slight oxidation of NO to NO₂, proportional to oxygen content, is discernible.

The 304 stainless steel probe (Figure 15b) catalytically reduces NO₂ to NO at temperatures in excess of 100°C. The conversion of NO₂ to NO at elevated temperatures is consistent with the results of a variety of studies in which stainless steel has been evaluated for use as the converter material in chemiluminescent nitrogen oxides analyzers.¹⁴⁻¹⁶ At temperatures below the catalytically active temperature of 200°C, no significant change is observed. The oxygen content of the mixture has an important impact on the conversion efficiency at the peak temperature evaluated (400°C).

The results for the 316 stainless steel, presented in Figure 15c, indicate that a higher temperature (>300°C) is required to initiate the catalytic reduction of NO₂ in comparison to 304 stainless steel. At 400°C, however, dissociation is nearly 100% complete. The oxygen content of the mixture has a modest impact on the conversion efficiency at the peak temperature evaluated (400°C). Slight evidence of oxidation of NO to NO₂ is again discernible at the lower temperatures.

The results for the 321 stainless steel, presented in Figure 15d, show behavior similar to the 316 stainless steel.

The three stainless steels evaluated have similar carbon, chromium, and nickel content.¹⁷⁻¹⁹ As shown in Table VI, however, 316 stainless steel has molybdenum added to improve corrosion resistance, and 321 stainless steel has titanium added to reduce carbide precipitation. In general, stainless steels have strong resistance to corrosion due to an oxidized layer on the surface. Reducing atmospheres can remove the oxide film and change the passivity. It is likely that prior exposure of stainless steel probes to varying sample environments may alter the degree of NO_x transformations. Evidence of probe history effects have been reported in the literature,²⁰ but a full assessment has yet to be made.

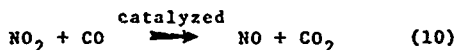
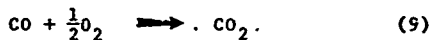
RESULTS (WITH CARBON MONOXIDE)

The results for silica are presented in Figure 16a. No significant transformation is observed at temperatures below 300°C. The slight oxidation of NO to NO_2 observed without carbon monoxide is not discernible when carbon monoxide is present. At 400°C some reduction of NO_2 to NO occurs. The reduction is dependent on both oxygen content as well as carbon monoxide level. At the level of carbon monoxide for which the transformation is most pronounced (2500ppm CO), the dependency on oxygen is the reverse of the dependency at lower carbon monoxide levels (100, 1000ppm CO).

The results for 316 stainless steel are presented in Figure 16b (304 and 321 stainless steels were not evaluated). The presence of carbon monoxide effectively lowers the temperature at which reduction of NO_2 to NO is observed. Significant reduction is observed at temperatures in excess of 100°C . The reduction is more pronounced as carbon monoxide is increased. Increased oxygen content has the effect of reducing the conversion at a given temperature and a given carbon monoxide level.

DISCUSSION

The results without carbon monoxide are expected and explainable by the known catalytic performance of stainless steel in reducing NO_2 to NO .¹⁴⁻¹⁶ The results with carbon monoxide are new and will require further testing to fully assess the controlling mechanism. Nevertheless, tentative explanations are possible by considering the competition between the following two reactions:



Increased CO will advance the reduction of NO_2 by reaction (10) as observed experimentally. Increased O_2 will inhibit the advance of reaction (10) due to the competition between O_2 and NO for the CO . In studies of CO oxidation by NO and O_2 , oxygen

is observed to preferentially oxidize CO to CO_2 .²¹⁻²³

The silica results with carbon monoxide indicate that reaction (10) may be active at 400°C. The advance of reaction (10) as a homogeneous reaction at 400°C is slow relative to the one second residence time. The dependency upon oxygen is not explained.

The results of Figure 16b (316 stainless steel with carbon monoxide) differ from an earlier investigation by Halstead²⁴ in that total oxides of nitrogen are conserved in the present study. The removal of NO_x observed by Halstead may result from (1) the reduction of NO_x by reducing species other than CO (e.g. hydrocarbons) present in the fuel rich flames sampled, (2) the elevated ($\approx 800^\circ\text{C}$) temperatures to which the samples were temporarily exposed at the probe inlet, (3) the longer residence time (4 seconds compared to 1 second) or (4) a combination. Further study that addresses additional reducing species, higher temperatures ($> 400^\circ\text{C}$), and longer residence times (> 1 second) will be necessary to fully assess the difference.

CONCLUSIONS

- Nitrogen oxides are sampled from combustion sources for a variety of reasons and over a wide range of temperatures and gas composition.
- A number of reactions are potentially active to transform nitrogen oxides concentration while sampling

combustion products.

- NO_x is conserved in silica and 304, 316, and 321 stainless steel sample probes for the temperature range 25 to 400°C and a residence time of 1 second.
- In the absence of carbon monoxide, reduction of NO_2 is observed in 316 and 321 stainless steel at temperatures exceeding 300°C. In 304 stainless steel, NO_2 reduction is observed at temperatures exceeding 100°C.
- In the presence of carbon monoxide, the reduction of NO_2 occurs at temperatures exceeding 100°C in 316 stainless steel.
- In silica, no significant transformation of nitrogen oxides is observed in the absence of carbon monoxide. When carbon monoxide is present at levels exceeding 1000ppm, reduction of NO_2 is observed at temperatures exceeding 300°C.
- Previous NO_x , NO and NO_2 data collected at moderate temperatures (25 to 600°C) with stainless steel sampling lines and at temperatures above 300°C with silica must be used with caution.
- The potential for chemical transformation of nitrogen oxides concentration while sampling combustion products at moderate temperatures may be reduced by (1) using only silica, (2) maintaining the temperature below 300°C in carbon monoxide containing atmospheres, and (3) exercising appropriate precaution in handling water in the sample

- Additional information is needed to assess the extent of chemical transformation that occurs under the variety of sampling conditions experienced in practice, and, guide the selection of probe and sample line materials in order to prevent the occurrence of chemical transformation.

3.5 Publications/Papers Presented

Two publications were submitted during the reporting period and three papers were presented. Papers are now in preparation or planned for publication or presentation. The current status of the publications and presentations of papers is summarized in Table VII.

4. DESCRIPTION OF RESEARCH DIRECTION:

CONTINUATION YEAR

4.1 Model Development and Evaluation

In the continuation year, the emphasis will be placed on the evaluation of the predictive methods for the case of heated (nonreacting) flow and hot (reacting) flow. The sensitivity study for initial and boundary conditions for the case of isothermal (nonreacting) flow will be completed as well.

Heated Flow. The heated case is designed to test the coupled submodels of eddy viscosity, mass transport, and energy transport. The heated flow case was initiated during the current reporting period with the design and installation of a preheat system into the combustion facility.

Hot Flow. The hot flow case will substantially increase the complexity of the evaluation. The added considerations include chemistry submodels (including the effects of turbulence on chemical reaction rates), and radiation submodels. Predicted profiles of velocity, turbulence kinetic energy, equivalence ratio, temperature and concentrations of hydrocarbons, oxygen, carbon monoxide, nitric oxide, nitrogen dioxide, and carbon dioxide will be compared to experimental results. Comparison of the predicted distributions to those determined experimentally will be used to identify deficiencies in the models of turbulence and kinetics for the condition of reacting flow.

The hot flow case was initiated during the past year by

(1) generating first solutions for the hot flow case (Figures 12 and 13), (2) generating hot flow experimental data for methane/air, and (3) preparing and submitting a proposal to the National Science Foundation for support to complement the hot flow evaluation studies.

4.2 Mechanisms of Pollutant / Plume Formation

The experimental studies designed to specifically explore the mechanism of pollutant and plume formation will commence in the summer of 1976. The experiment will be used alone and in combination with numerical results in the next twelve month period to explore pollutants and plume formation. Parametric studies will be conducted to establish the relative effect of the transport and chemical processes (chemical kinetics, mass and heat diffusion, and fluid mechanics) and system parameters (jet and main stream flow rates, composition, temperature, size and shape of the recirculation zone) on pollutant formation.

4.3 Supplemental Studies

Under supplemental studies, the exploration of the lean stabilized combustion performance of the OJC will be initiated and completed, the air preheat studies will continue, a nonpremixed combustor configuration will be designed and tested to complement the premixed OJC geometry, swirl will be added, the NO probe study will be expanded to explore a variety of hydrogen containing species and probe history, and studies will be initiated that address particulate formation and luminosity, especially in relation to the on-going alternative fuel studies at AFAPL. The supplemental studies have been added to specifically address current needs of the Air Force.

5. SUMMARY

The UCI investigation of exhaust pollutant and plume formation in continuous combustion is a combined analytical and experimental study of turbulent, backmixed combustion. Predicted profiles of the flow properties are being systematically compared to experimentally determined profiles. Model development and evaluation, and studies of the mechanisms of pollutant and plume formation are being conducted for premixed methane/air and propane/air reactants.

Future work will include nonpremixed combustion and a liquid fuel system.

5.1 Model Development and Evaluation

Nonreacting. The isothermal evaluation of the PISTEP II and TEACH numerical codes has addressed the effective viscosity and mass transport submodels. Still to be completed is a thorough investigation of initial and boundary conditions.

The heated flow evaluation has been initiated by the design and installation of preheat capability. The evaluation will conclude during the continuation year.

In cooperation with the EPA, the CRISTY numerical code is being run as time permits in parallel with the PISTEP II and TEACH numerical codes. The interaction is proving useful to both parties (UCI/AFOSR and EPA), and comparative results will likely be available for presentation in the continuation year.

Reacting. Hot flow solutions have been obtained with TEACH

and the numerical codes (TEACH and PISTEP II) are currently being expanded to include propane kinetics. Initial experimental data have been obtained in preparation for the coupled numerical/experimental evaluation in the continuation year.

5.2 Mechanisms of Pollutant/Plume Formation

The experimental facility is undergoing final modification (inclusion of preheat capability) prior to initiating the scheduled exploration of the mechanisms responsible for pollutant and plume formation in continuous combustion. To improve the signal aquisition of the LDV System, the addition of a counter mode to complement the existing frequency tracking mode is under investigation. The sampling performance of the combustion test facility is being improved as a result of the supplementary, NO probe studies.

5.3 Supplementary Studies

The NO probe study has shown significant reduction of nitrogen dioxide (NO_2) to nitric oxide (NO) can occur in sample probes and sample lines, especially in the presence of carbon monoxide (CO) at modest temperatures in stainless steel. The effects of probe history and reducing species in addition to CO will be evaluated in the continuation year. In addition, lean combustion emission, air preheat, non-premixed, swirl, and particulate/luminosity studies will be initiated.

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TABLE I

Elliptic Flow Codes

CODE	PRINCIPAL VARIABLES	ORIGINATOR	REFERENCE
PISTEP11	$\phi - \omega$	Imperial College London	3,25
TEACH	$P - v$	Imperial College London	26
CRISTY*	$\psi - \omega$	United Technology Research Center Connecticut	27,28

* Earlier versions called FNEP and GFREP

TABLE II

Emission Instrumentation

Carbon Monoxide Analyzer (Beckman 315BL NDIR)
Range: 0-100ppm, 0-500ppm, 0-2500ppm
0-1%, 0-10%

Carbon Dioxide Analyzer (Beckman 315A NDIR)
Range: 0-2%, 0-5%, 0-15% CO₂

Oxides of Nitrogen Analyzer (Scott 125 Chemiluminescence)
Range: 0-1, 0-5, 0-10, 0-50, 0-100, 0-500, 0-1000
0-5000, 0-10000ppm NO-NO_x

Oxygen Analyzer (Scott 150 paramagnetic)
Range: 0-1%, 0-5%, 0-10%, 0-25% O₂

High Temperature Total Hydrocarbon Analyzer (Scott 215FID)
Range: 0-1, 0-5, 0-10, 0-50, 0-100, 0-500, 0-1000,
0-5000, 0-10000, 0-50000, 0-100000ppm HC

All instrument specifications indicate an accuracy of $\pm 1\%$
full scale

TABLE IV

Predictive Methods

Improvements/Modifications During Reporting Period

Following is a description of tasks which required either modification of existing methods or new developments

TFACH

1. Isothermal flow - submodels for momentum and mass transport tested against experiment. Improved boundary conditions required.
2. Hot flow - solution obtained for methane oxidation including formation of nitric oxide.

PiSTEP II

1. Isothermal flow - tests of submodels for momentum and mass transport against experiment initiated. Evidence of boundary condition modification observed.

CRISTY

1. Isothermal flow - successfully modified for UCI OJC geometry in cooperation with the EPA. Tests against experiment initiated.

Following is a description of remaining problems and plans for their resolution.

TEACH, PiSTEP II, CRISTY

No problems are current excluding the chronic demand of numerical work for additional resources. The development and evaluation of the numerical codes are modestly behind schedule, but the present rate of progress and success in securing additional resources will return the development and evaluation to the planned schedule.

TABLE V

Combustor Test Facility

Improvements/Modifications During Reporting Period

Following is a description of tasks which required either modification of existing equipment or new work to be performed.

1. Inlet air flow preheat - to more effectively simulate gas turbine combustion and explore the effect of air preheat on numerical model development and evaluation and pollutant/plume formation, air preheat capability was added. Inlet temperatures to 600°C (1112°F) are now available.
2. Exhaust heat load - an air dilution system and water cooled heat exchanger coil were installed to allow higher combustor loadings to be accommodated without thermally taxing the building exhaust system.
3. Sample probe - a 1/8-inch O.D. sample probe was designed, built, tested, and used for composition measurements. The 1/8-inch size reduced the impact on the flowfield of the previous, 1/4-inch probe.
4. Emission Console overhaul - the emission console was thoroughly inspected and serviced prior to the generation of the data base runs. All tubing was disconnected, cleaned, and reassembled.
5. Data Acquisition System - the DEC PDP-11 data acquisition system was installed and successfully interfaced with the combustor facility instrumentation. All necessary software has been developed, checked and is currently in operation.

Following is a description of remaining problems and plans for their resolution.

1. Combustor Size - the 51mm (2-inch) I.D. combustor size has proven adequate for the studies conducted but not optimum for the resolution desired for property profile measurements. A 76mm (3-inch) combustor section has been designed and is currently being fabricated. The flexibility of changing combustor size will prove useful in evaluating boundary condition impact on the numerical codes.
2. Sample probe design - studies conducted to explore chemical transformation of nitrogen oxides in probes and lines have shown that stainless steel will catalytically reduce NO_x to NO in the presence of CO at temperatures in excess of 100°C. A silica, water coated sampling probe is equipped with aerodynamic quench, is currently being designed.
3. Swirl - swirl is an integral factor in promoting plume stabilization in practical, continuous combustion devices. The numerical methods must be tested for the case of swirl as well as non-swirl if successful simulations of practical devices are to be achieved. Swirl vanes are currently being designed.
4. LDV System - the performance of the frequency tracker deteriorates to unacceptable levels in the highly turbulent region of jet penetration. Seeding techniques for the jet and expansion of the signal acquisition system to include the counter mode are being explored.

TABLE VI
Stainless Steel Composition^a

TABLE VI Stainless Steel Composition ^a						
Specification	S.S. Type	Typical Weight Percent				
		Carbon	Chromium	Nickel	Molybdenum	Titanium
General ¹⁷	304	0.08	18-20	8-12		
	316	0.08	16-18	10-14	2-3	
	321	0.08	17-19	9-12		0.40
Present Study ^{18,19}	304	0.03	18.12	8.64		
	316	0.004	17.60	12.43	2.72	
	321	0.065	17.75	10.78	0.30	0.47

^a Other elements present include manganese, phosphorus, sulfur, silica, copper

TABLE VII

Publications and Presentation of Papers

Publications	Presentation of Papers
<p><u>Submitted</u></p> <p>Eddy Viscosity Modeling in the Prediction of Turbulent, Batched Combustion Performance</p> <p>Sixteenth (International) Symposium on Combustion</p> <p>Chemical Transformations of Nitrogen Oxides in Sample Probes and Sample Lines While Sampling Combustion Products</p> <p>Journal Air Pollution Control Association</p> <p>Analytical and Experimental Study of Turbulent Methane - Fired Batched Combustion</p> <p>AIChE Journal</p>	
<p><u>Accepted</u></p>	<p>Eddy Viscosity Modeling in the Prediction of Turbulent, Batched Combustion Performance</p> <p>Sixteenth (International) Symposium on Combustion August, 1976</p>
<p><u>Presented</u></p>	<p>Analytical and Experimental Study of Turbulent Methane - Fired Batched Combustion</p> <p>AIChE/SAE 11th Propulsion Conference Anaheim, California, September, 1976</p> <p>Transformation of Oxides of Nitrogen While Sampling Combustion Products</p> <p>First International Chemical Congress, ACS Mexico City, December, 1975</p> <p>Oxides of Nitrogen Transformation While Sampling Combustion Products Containing Carbon Monoxide</p> <p>1976 Spring Meeting Western States Section/Combustion Institute University of Utah April, 1976</p>
<p><u>Planned</u></p> <p>Extension Characteristics of a Lean Aerodynamic Stabilized Methane - Fired Combustor</p> <p>Submission: December 1976</p> <p>Mass Transport Modeling in the Prediction of Turbulent, Batched Combustion Performance</p> <p>Effect of Preheat on the Extension Characteristics of an Aerodynamic Stabilized Propane-fired Combustor</p> <p>Submission: October 1976</p> <p>Pollutant Formation in Recirculating Flows</p> <p>Submission: February 1976</p>	<p>Oxides of Nitrogen Transformation While Sampling Combustion Products Containing Hydrogen</p> <p>1976 Fall Meeting Western States Section/Combustion Institute University of California, San Diego October 1976</p>

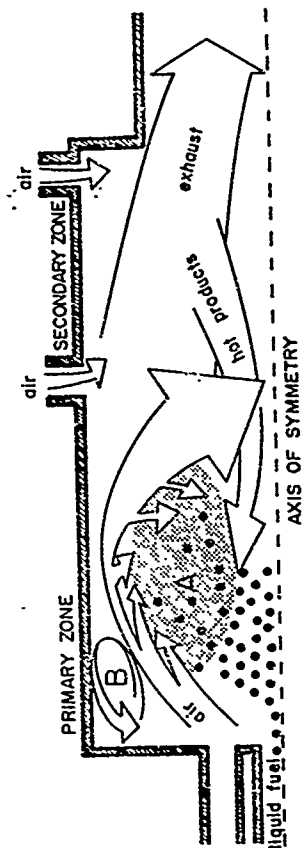


Figure 1 Schematic of Gas Turbine Combustor

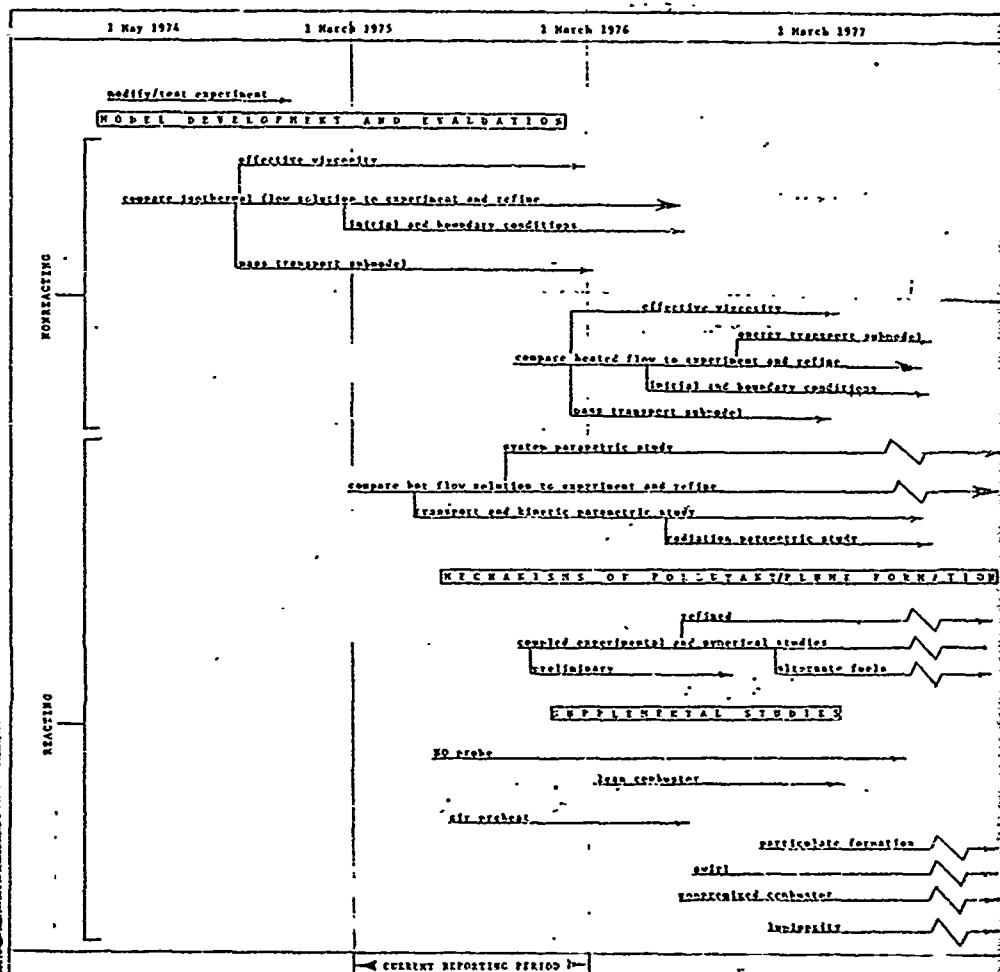


Figure 2 Performance Schedule

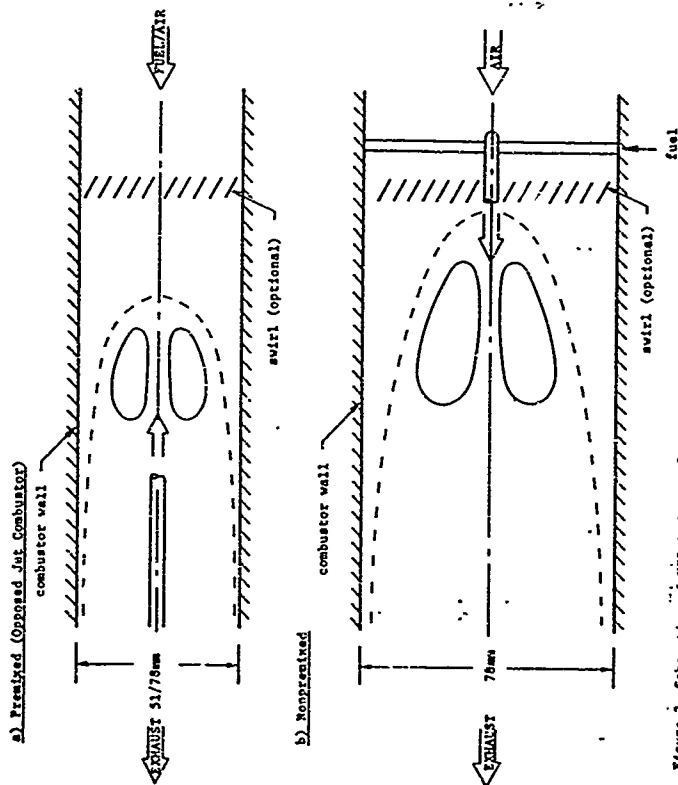


Figure 3 Schematic of UCI Combustor Systems

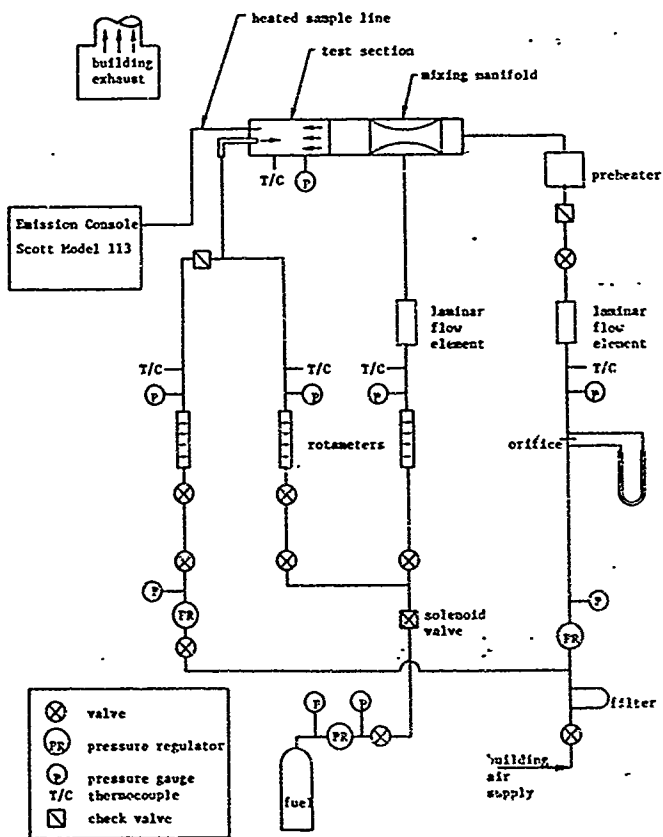


Figure 4 Flow Diagram - Combustor Test Facility

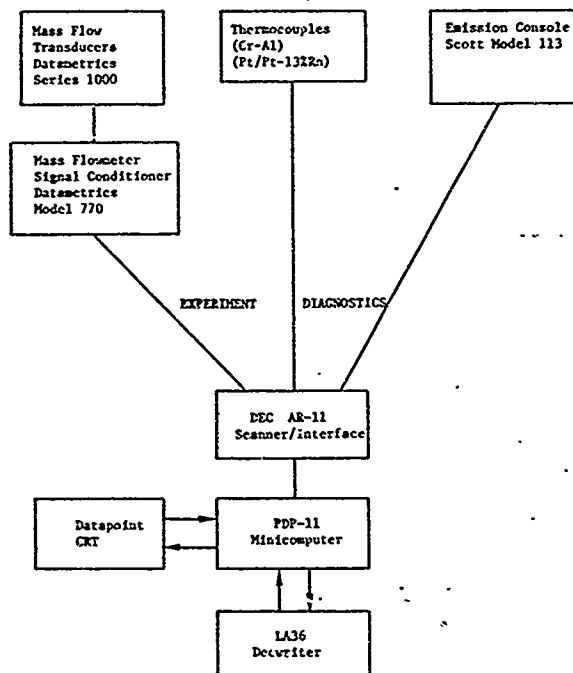
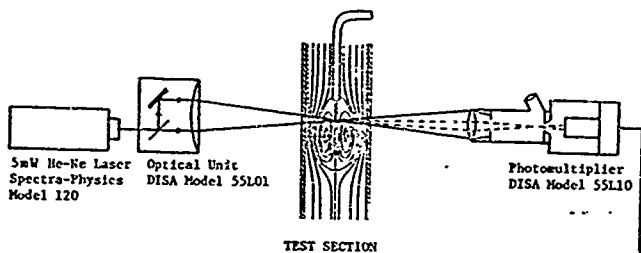


Figure 5 PDP-11 Data Acquisition System

• Optical Arrangement



• Signal Processing Electronics

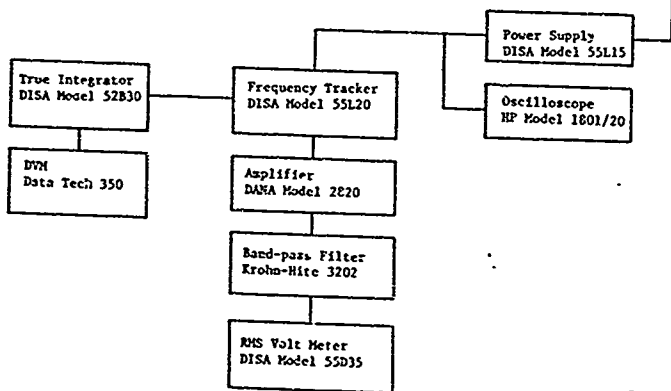


Figure 6 LDV System Components

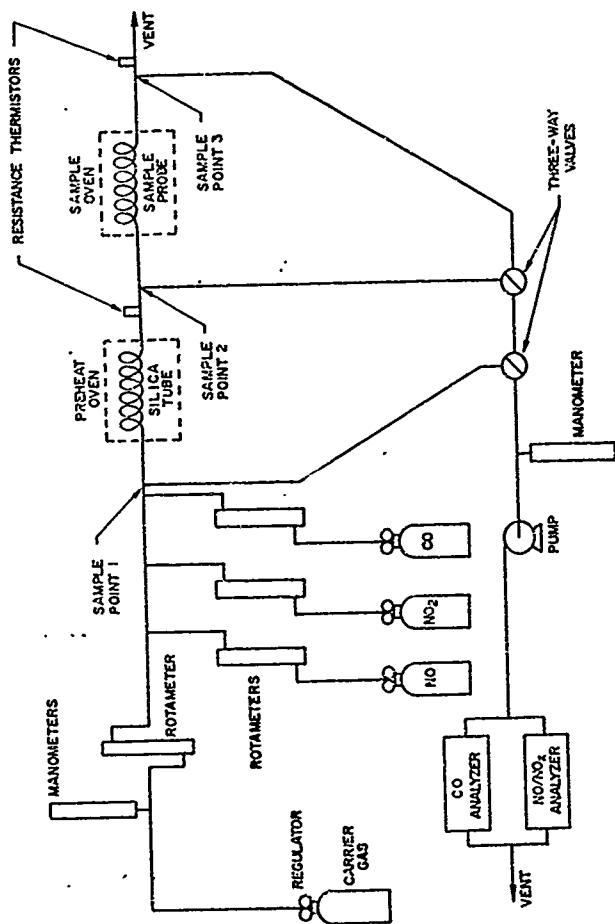


Figure 7 Flow Diagram - NO Probe Test Facility

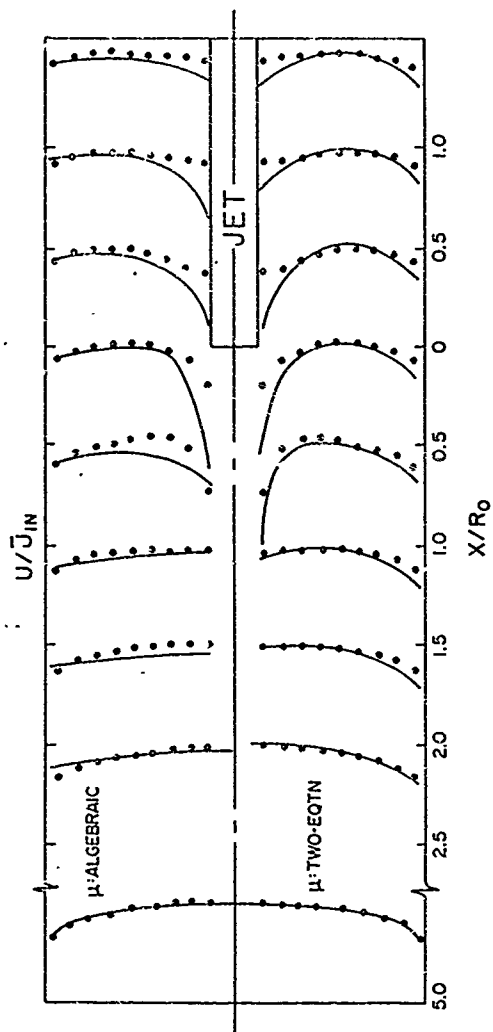


Figure 8 Isothermal Flow Velocity Profiles (— predicted, \circ experimental); $\bar{U}_m = 15.24\text{m/sec}$; $\bar{U}_j = 130\text{m/sec}$; $\phi_m = \phi_j = 0$

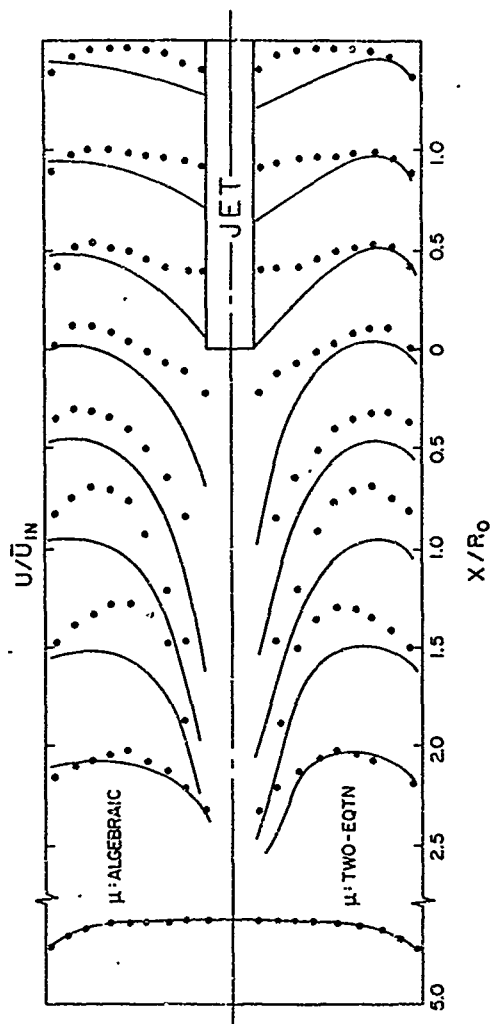


Figure 9 Isothermal Flow Velocity Profiles (— predicted, \circ experimental); $\bar{U}_m = 7.62\text{m/sec}$; $\bar{U}_j = 130\text{m/sec}$; $\phi_m = \phi_j = 0$

a) μ :algebraic

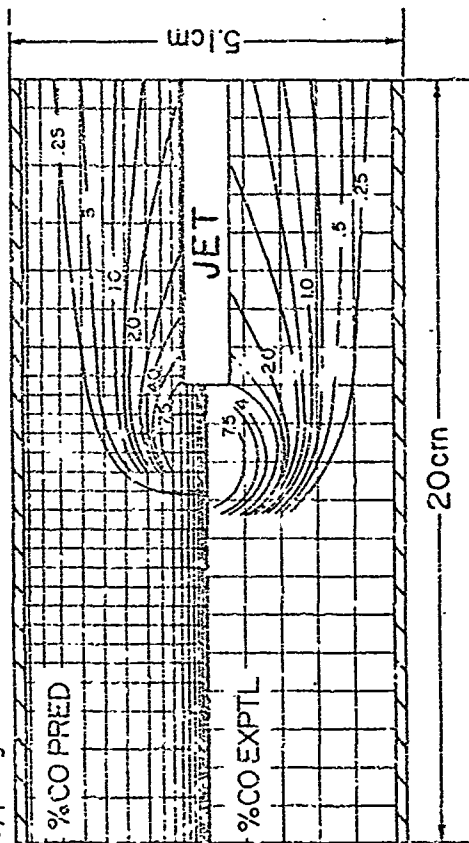


Figure 10 Isothermal Flow Tracer Concentration Profiles¹¹
 $U_m = 15.24 \text{ m/sec}$; $U_j = 150 \text{ m/sec}$; $\phi_m = 0.1$ 100 ft CO Jet

b) μ : two-equation

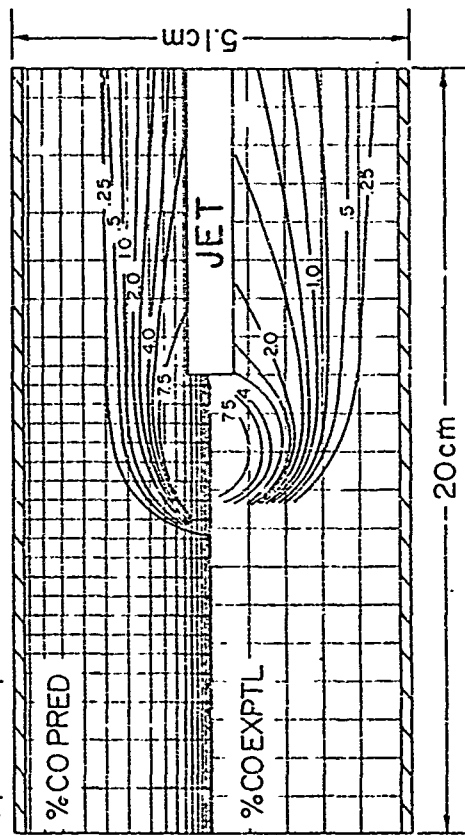


Figure 10 (con't)

a) μ : algebraic

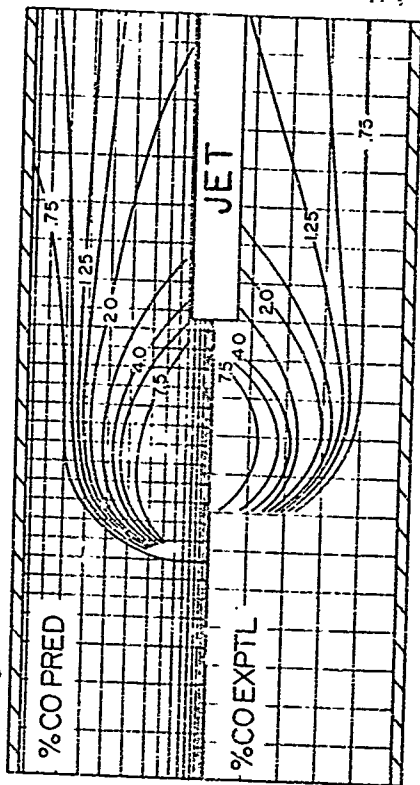


Figure 11 Isothermal Flow Tracer Concentration Profiles:
 $U_m = 7.62 \text{ m/sec}$; $U_j = 130 \text{ m/sec}$; $\phi_m = 0.1$ 100% CO Jet

b) μ : two-equation

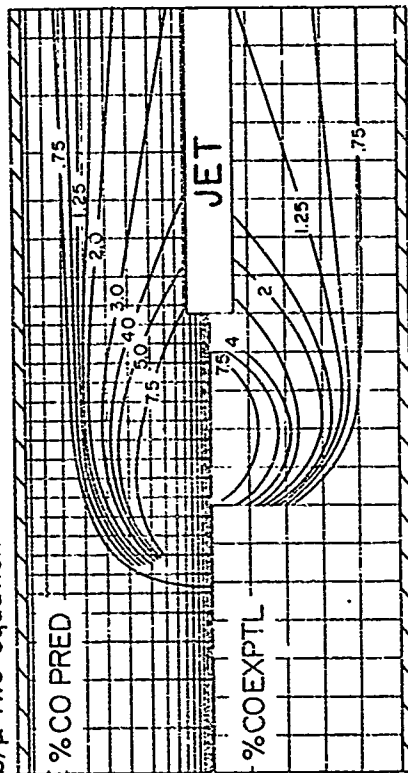


Figure 11 (con't)

a) μ : algebraic

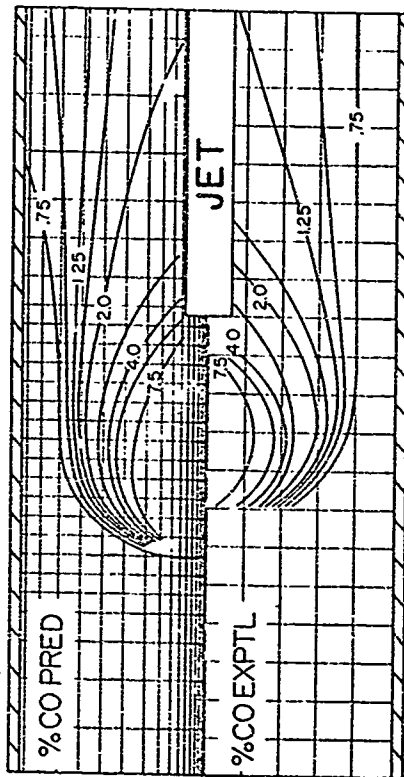


Figure 11 Isothermal Flow Tracer Concentration Profiles;
 $U_m = 7.62\text{m/sec}$; $U_j = 130\text{m/sec}$; $\phi_m = 0.1$ 100% CO Jet

a) μ : algebraic

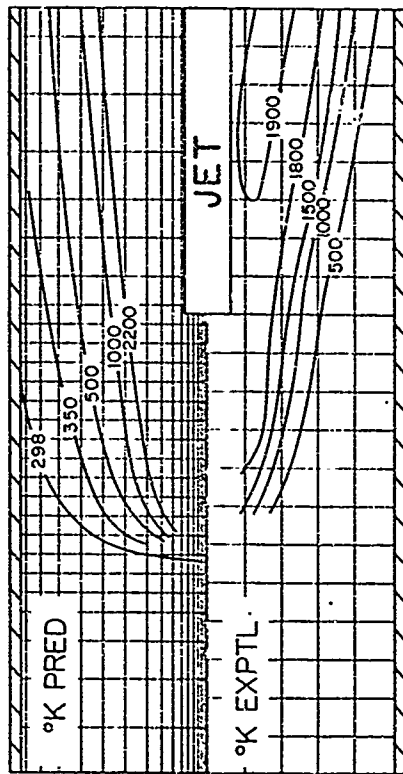


Figure 12 Hot Flow Temperature Distribution¹⁹
 $\bar{u}_m = 15.2 \text{ m/sec}$; $\bar{u}_j = 130 \text{ m/sec}$; $\phi_m = \phi_j = 1.0$.

b) μ : two-equation

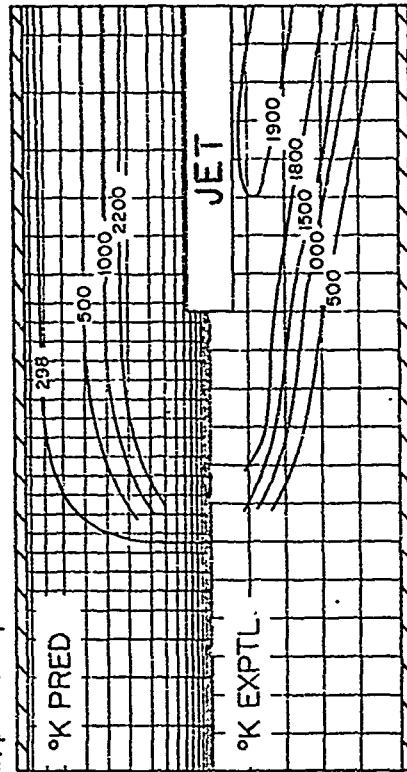


Figure 12 (cont.)

a) μ : algebraic

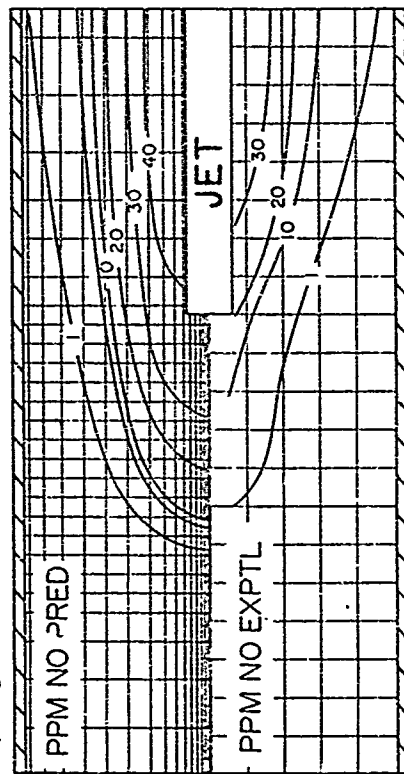


Figure 13 Hot Flow Nitric Oxide Concentration Profiles:
 $\bar{u}_m = 15.24m/sec$; $\bar{u}_j = 130m/sec$; $\phi_m = \phi_j = 1.0$.

b) μ : two-equation

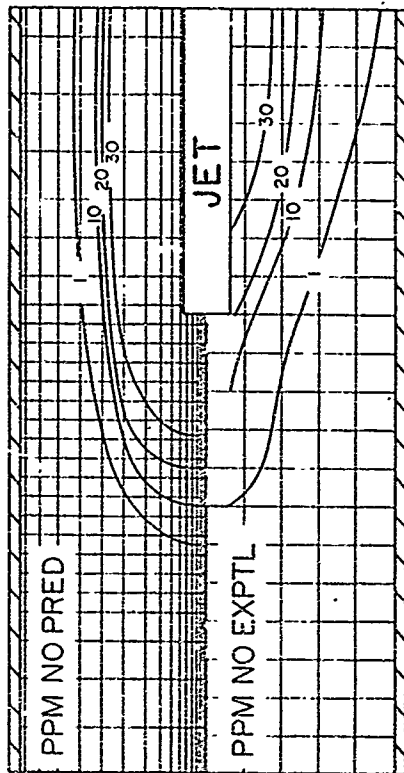


Figure 13 (con't)

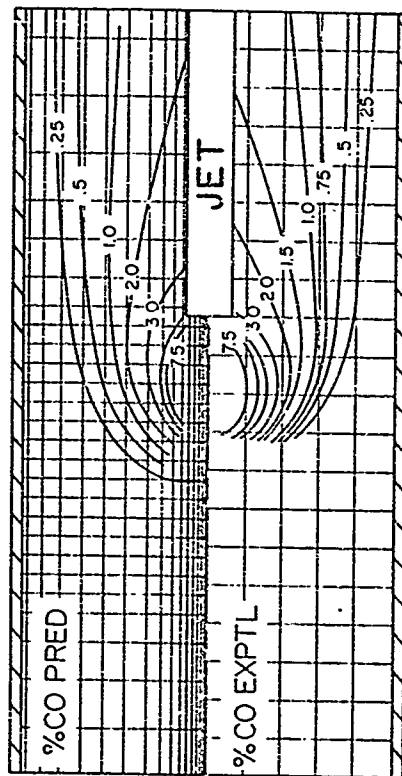


Figure 14 Isothermal Flow Tracer Concentration Profiles for Refined Jet Boundary Conditions (for two-equation) : $U_j = 15.24\text{m/sec}$; $U_m = 150\text{m/sec}$; $\phi_m = 0.1$ 100% Jet

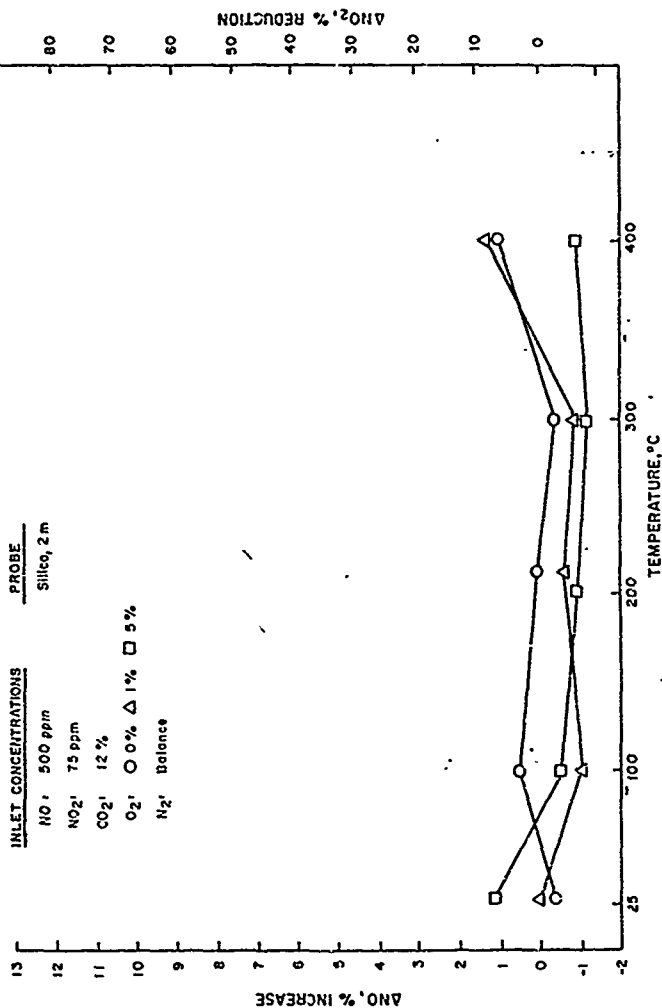


Figure 15a NO_x Transformation - Silica Test Probe

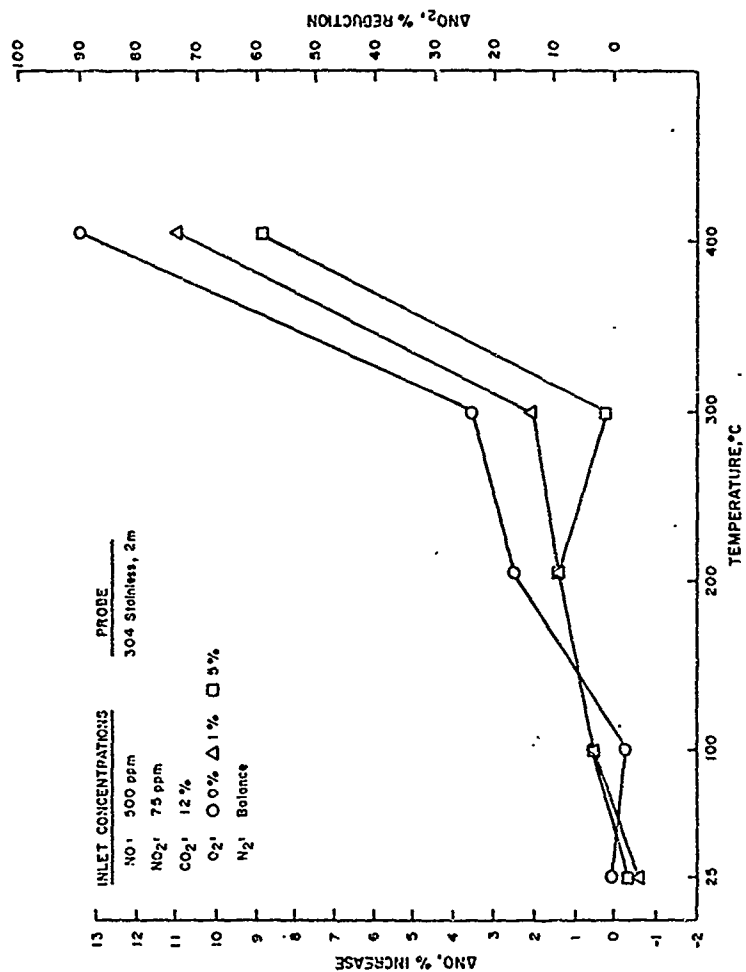


Figure 13b NO_x Transformation - 304 Stainless Steel Test Probe¹²

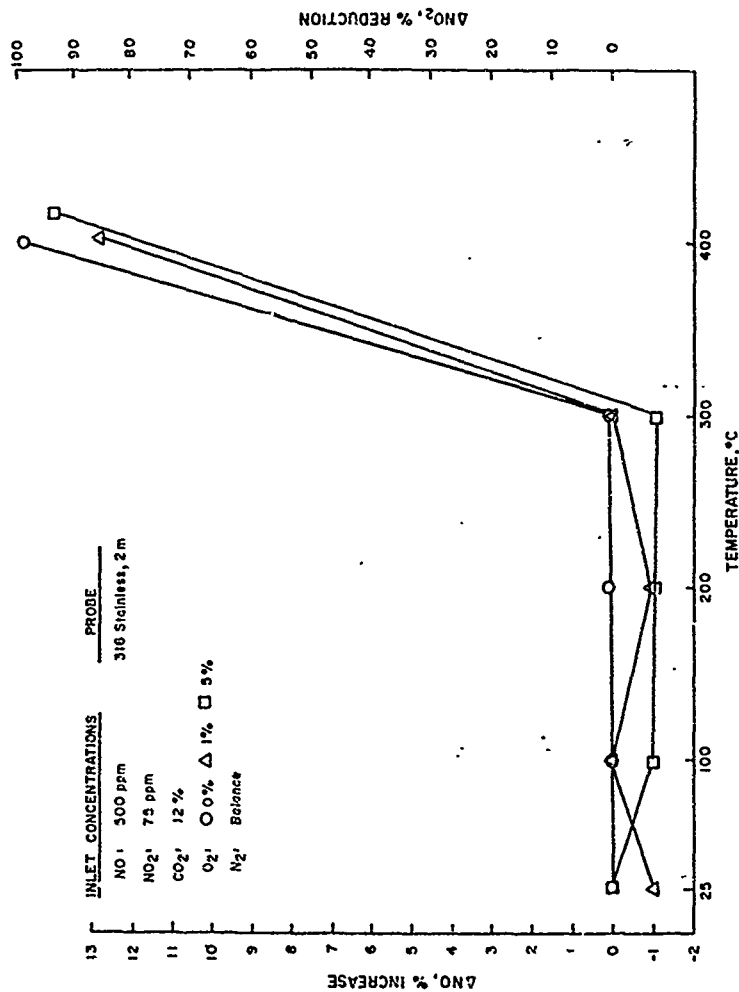


Figure 13c NO_x Transformation - 316 Stainless Steel Test Probe^{1,2}

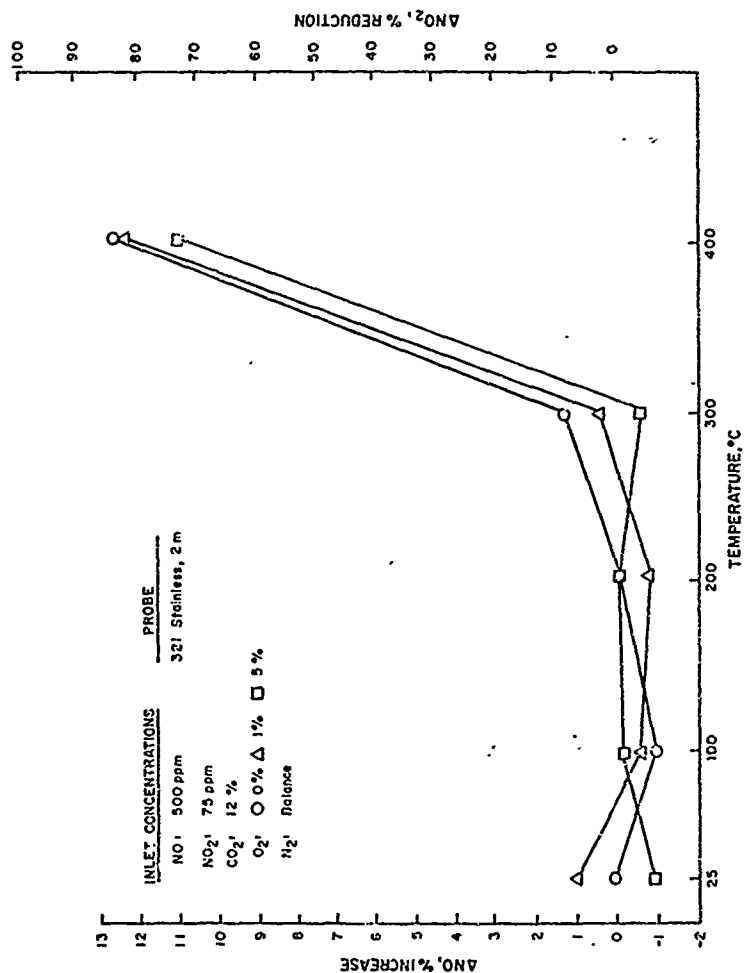


Figure 15d NO_x Transformation - 321 Stainless Steel Test Probe 12

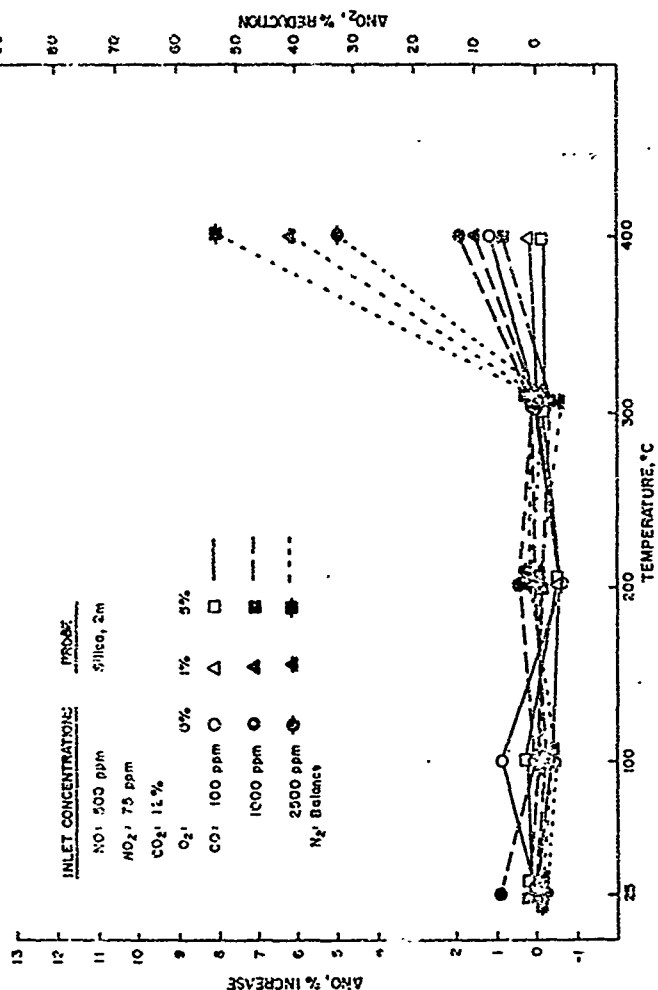


Figure 10a NO_x Transformation - Silica Test Probe

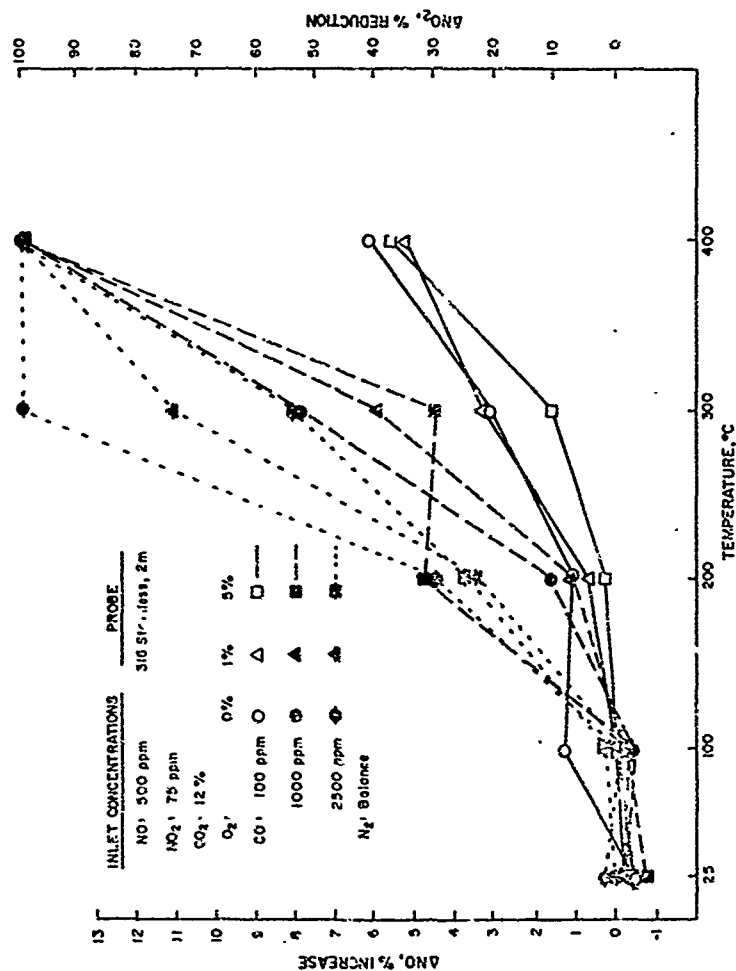


Figure 16b NO_x Transformation - 316 Stainless Steel Test Probe